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Crystal and molecular structure of two insecticides: Amido-o, s-dimethylthiophosphate and n-acetamido- o, s-dimeth ylthiophosphate

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Abstract

The crystal and molecular structure of title compounds have been determined by means of X-ray analysis. The amido-O.S-dimethylthiophosphate (1) crystallizes in the monoclinic space group P21/n with cell dimensions a = 5. 374(3), b = 9. 220(4), c = 13.847(5) Å and β = 101.08(5)° at the - 100°C. The N-acetamido-O.S-dimethylthiophosphate (2) crystallizes in the monoclinic space group P21/c with cell dimensions a = 11. 547(3), b = 8. 545(2), c = 8.954(5) Å and β = 93.03(4)°. The structures were solved by direct methods and refined by least-squares to R = 0. 0493(1) and 0.0482(2). The coordination around P of the molecules (1) and (2) is distorted tetrahedrally. Molecules have nearly planar moieties HCSP=O and HNPOC (1), HCSP=O and HCC (0) NHPOC (2) with trans-orientation HCSP, CSP=O and NPOC groups. The angle between these planes is 85.3° (1) and 90.3° (2). There are intermolecular P=O ... H-N hydrogen bonds in the crystal structures (1) and (2).

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Keywords

Amidothiophosphates, crystal structure, insecticides